

Towards computability of trace distance discord

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It is known that a reliable geometric quantifier of discord-like correlations can be built by employing the so-called trace distance. This is used to measure how far the state under investigation is from the closest “classical-quantum” one. To date, the explicit calculation of this indicator for two qubits was accomplished only for states such that the reduced density matrix of the measured party is maximally mixed, a class that includes Bell-diagonal states. Here, we first reduce the required optimization for a general two-qubit state to the minimization of an explicit two-variable function. Using this framework, we show next that the minimum can be analytically worked out in a number of relevant cases including quantum-classical and X states. This provides an explicit and compact expression for the trace distance discord of an arbitrary state belonging to either of these important classes of density matrices.

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I. INTRODUCTION

The issue that the quantum correlations (QCs) of a composite state are not entirely captured by entanglement (as formerly believed) has recently emerged as a topical subject calling for the introduction of new paradigms. Despite early evidence of this problem was provided over a decade ago [2] an impressive burst of attention to this matter has developed only in the last few years [1]. In this paper, we focus on those correlations that are associated to the notion of *quantum discord* [2]. Following the introduction of this concept, a variety of different measures of QCs have been put forward (see Ref. [1] for a comprehensive review). A major reason behind such a proliferation of QCs indicators stems from the typical difficulty in defining a reliable measure that is easily computable. No general closed formula of quantum discord, for instance, is known (with strong indications that this is an unsolvable problem [4]) even for a pair of two-dimensional systems or “qubits” [3], namely the simplest composite quantum system. Unfortunately, the demand for computability typically comes at the cost of ending up with quantities that fail to be *bona fide* measures. In this respect, the most paradigmatic instance is embodied by the so called *geometric discord* (GD) [5], which while being effortlessly computable (and in some cases able to provide useful information) suffers from a major drawback. It can indeed grow under local operations on the unmeasured party [6], an effect which a bona fide indicator (e.g. quantum discord) is required not to exhibit. Following an approach frequently adopted for other QCs measures, the one-sided GD is defined as the distance between the state under study and the set of classical-quantum states. The latter class features zero quantum discord with respect to the measured party, say subsystem A , which entails the existence of at least one set of local projective measurements on A leaving the state unperturbed [2, 7]). While the above definition in terms of a distance is clear and intuitive, it requires the use of a metric in the Hilbert space. The GD employs the Hilbert-Schmidt distance, which is defined in terms of the Schatten 2-norm.

Such a distance is well-known not to fulfill the property of being contractive under trace-preserving quantum channels [8], which is indeed the reason behind the aforementioned drawback of GD [9]. This naturally leads to a redefinition of the GD in terms of a metric that obeys the contractivity property. One such metric is the *trace distance* [3], which employs the Schatten 1-norm (or trace norm for brevity). In the remainder of this paper, we refer to the QCs geometric measure resulting from this specific choice as *trace distance discord* (TDD).

While investigations are still in the early stages [10–14], TDD appears to enjoy attractive features. Besides the discussed contractivity property, the trace distance is invariant under unitary transformations. More importantly, it is in one-to-one correspondence with *one-shot state distinguishability* [15], i.e., the maximum probability to distinguish between two states through a single measurement. This operational interpretation provides evidence that the trace distance works as an accurate “meter” in the space of quantum states. Another appealing advantage of TDD lies in its connection with entanglement. Recently, indeed, it was suggested to define the full amount of discord-like correlations in a system S as the minimum entanglement between S and the measurement apparatus created in a local measurement (see [16–18] and references therein). This way, a given entanglement measure [19] identifies a corresponding QCs indicator. Remarkably, it turns out that the latter always exceeds the entanglement between the subparts of S when this is quantified via the same entanglement measure. This rigorously formalizes the idea that a composite state can feature QCs that cannot be ascribed to entanglement. In this framework, it can be shown [12] that the entanglement counterpart of TDD is *negativity* [20], the latter being a well-known – in general easily computable – entanglement monotone [21].

In spite of all such interesting features, the easiness of computation of TDD in actual problems is yet to be assessed. To date, the only class of states for which a closed analytical expression has been worked out are the Bell-diagonal (BD) two-qubit states, or more generally states that appear maximally

mixed to the measured party [12, 13]. While the proof of this formula is non-trivial [12], this does not clarify whether or not, besides its reliability, TDD brings about computability advantages as well. Owing to the high symmetry and reduced number of parameters of BD states, indeed, most if not all of the bona fide QCs measures proposed so far can be analytically calculated for this specific class [23].

In this paper, we take a step forward and set up the problem of the actual computation of two-qubit TDD on a new basis. We first develop a theoretical framework that reduces this task to the equivalent minimization of a two-variable explicit function, which parametrically depends on the Bloch vectors of the marginals and the singular values of the correlation matrix. Next, after re-deriving the value of TDD for a class of density matrices that includes BD states, we discuss two further relevant cases in which the minimization problem can be analytically solved. One is the case where the correlation matrix has one non-zero singular eigenvalue, a subset of which is given by the *quantum-classical* states (unlike classical-quantum states these feature non-classical correlations with respect to party A). The other case is given by the family of *X states* [22], which include BD states as special cases. While these are arguably among the most studied classes of two-qubit density matrices [1], the calculation of their QCs through bona fide measures is in general a demanding task. To the best of our knowledge, in particular, no closed expression for an arbitrary quantum-classical state is known to date with the exception of Ref. [24] where however an *ad hoc* measure exclusively devised for this specific class of states was presented. In the general case, indeed, one such state depends on four independent parameters and, moreover, features quite low symmetry. In Refs. [24] and [25], for instance, closed expressions for a fidelity-based measure [26] and the quantum discord, respectively, could be worked out only for high-symmetry two-parameter subsets of this family.

Even more involved is the calculation of QCs in the case of *X states*, a class which depends on five independent parameters. Regarding quantum discord, an algorithm has been put forward by Ali *et al.* [27]. Later, however, some counterexamples of *X states* for which such algorithm fails were highlighted [28] (see also Ref. [1]).

The present paper is organized as follows. In Section II, we present our method for tackling and simplifying the calculation of TDD for an arbitrary two-qubit state. This is demonstrably reduced to the minimization of an explicit two-variable function. In Section III, we apply the theory to the case of Bell states and that of density matrices having correlation matrix with uniform spectrum. In Section IV, we show that the minimum can be analytically found in a closed form whenever the correlation matrix of the composite state features only one non-zero singular value. As an application of this finding, in Subsection IV A we compute the TDD of the most general quantum-classical state. As a further case where the minimization in Section II can be performed explicitly, in Section V we tackle the important class of *X states* and work out the TDD for an arbitrary element of this. We finally draw our conclusions in Section VI. A few technical details are presented in the Appendix.

II. ONE-SIDED TDD FOR TWO-QUBIT STATES: GENERAL CASE

The one-sided TDD $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$ from *A* to *B* of a bipartite quantum state ρ_{AB} is defined as the minimal (trace norm) distance between such state and the set *CQ* of *classical-quantum* density matrices which exhibit zero quantum discord with respect to local measurements on *A*, i.e. states which admit an unravelling of the form

$$\rho_{AB}^{(\rightarrow)} = \sum_j |\alpha_j\rangle_A \langle \alpha_j| \otimes \varrho_B(j) \quad (1)$$

with $|\alpha_j\rangle_A$ being orthonormal vectors of *A* and $\varrho_B(j)$ being positive (non necessarily normalized) operators of *B*. Specifically, if $\|\Theta\|_1 = \text{Tr}[\sqrt{\Theta^\dagger \Theta}]$ denotes the trace norm (or Schatten 1-norm) of a generic operator Θ then

$$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{1}{2} \min_{\{\rho_{AB}^{(\rightarrow)}\}} \|\rho_{AB} - \rho_{AB}^{(\rightarrow)}\|_1, \quad (2)$$

the 1/2 factor ensuring that $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$ takes values between 0 and 1 [analogous definition applies for the one-sided TDD from *B* to *A*, $\mathcal{D}^{(\leftarrow)}(\rho_{AB})$]. The quantity in Eq. (2) fulfills several requirements which make it fit for describing non-classical correlations of the discord type [12]. In particular, from the properties of the trace distance [3] it follows that $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$

i) is zero if and only if ρ_{AB} is one of the classical-quantum density matrices (1);

ii) is invariant under the action of an arbitrary unitary operation $U_A \otimes V_B$ that acts locally on *A* and *B*, i.e.

$$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) \equiv \mathcal{D}^{(\rightarrow)}(U_A \otimes V_B \rho_{AB} U_A^\dagger \otimes V_B^\dagger); \quad (3)$$

iii) is monotonically decreasing under completely positive and trace preserving (CPT) maps on *B*;

iv) is an entanglement monotone when ρ_{AB} is pure.

Furthermore, in the special case in which *A* is a qubit Eq. (2) can be expressed as [12]

$$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{1}{2} \min_{\{\Pi_A\}} \|\rho_{AB} - (\Pi_A \otimes \mathbb{1}_B)(\rho_{AB})\|_1, \quad (4)$$

where now the minimization is performed with respect to all possible completely depolarizing channel Π_A on *A* associated with projective measurements over an orthonormal basis, i.e.

$$\Pi_A(\cdots) = P_A \cdots P_A + Q_A \cdots Q_A, \quad (5)$$

with $P_A \equiv |\Psi\rangle_A \langle \Psi|$ and $Q_A = \mathbb{1}_A - P_A$ being rank-one projectors ($|\Psi\rangle$ is a generic one-qubit *pure* state).

In what follows, we will focus on the case where *both A and B* are qubits. Accordingly, we parametrize the state ρ_{AB}

in terms of the Pauli matrices $\vec{\sigma}_{A(B)} = \{\sigma_{A(B)1}, \sigma_{A(B)2}, \sigma_{A(B)3}\} \equiv \{\sigma_{A(B)x}, \sigma_{A(B)y}, \sigma_{A(B)z}\}$, i.e.

$$\rho_{AB} = \frac{1}{4}(\mathbb{1}_A \otimes \mathbb{1}_B + \vec{x}_A \cdot \vec{\sigma}_A \otimes \mathbb{1}_B + \mathbb{1}_A \otimes \vec{x}_B \cdot \vec{\sigma}_B + \sum_{i,j=1}^3 \Gamma_{ij} \sigma_{Ai} \otimes \sigma_{Bj}) \quad (6)$$

where

$$\vec{x}_{A(B)} = \text{Tr}[\rho_{AB} \vec{\sigma}_{A(B)}], \quad (7)$$

is the Bloch vector corresponding to the reduced density matrix $\rho_{A(B)}$ describing the state of $A(B)$, while Γ is the 3×3 real correlation matrix given by

$$\Gamma_{ij} = \text{Tr}[\rho_{AB} (\sigma_{Ai} \otimes \sigma_{Bj})]. \quad (8)$$

Similarly, without loss of generality, we express the orthogonal projectors P_A and Q_A of Eq. (5) as

$$P_A = \frac{1}{2}(\mathbb{1}_A + \hat{e} \cdot \vec{\sigma}_A), \quad Q_A = \frac{1}{2}(\mathbb{1}_A - \hat{e} \cdot \vec{\sigma}_A) \quad (9)$$

with \hat{e} being the 3-dimensional (real) unit vector associated with the pure state $|\Psi\rangle_A$ in the Bloch sphere. Using this and observing that $\Pi_A(\mathbb{1}_A) = \mathbb{1}_A$, and $\Pi_A(\vec{v} \cdot \vec{\sigma}_A) = (\hat{e} \cdot \vec{v})(\hat{e} \cdot \vec{\sigma}_A)$, Eq. (4) can be arranged as

$$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{1}{8} \min_{\hat{e}} \|M(\hat{e})\|_1, \quad (10)$$

where the minimization is performed over the unit vector \hat{e} and $M(\hat{e})$ is a 4×4 matrix which admits the representation

$$M(\hat{e}) = [(\vec{x}_A - (\hat{e} \cdot \vec{x}_A)\hat{e}) \cdot \vec{\sigma}_A] \otimes \mathbb{1}_B + \sum_{ij} \Gamma_{ij} (\hat{x}_i - e_i \hat{e}) \cdot \vec{\sigma}_A \otimes \sigma_{Bj}. \quad (11)$$

Here, \hat{x}_i is the i th Cartesian unit vector and $e_i = \hat{x}_i \cdot \hat{e}$ the i th component of \hat{e} (note that $\sigma_{Ai} = \hat{x}_i \cdot \vec{\sigma}_A$). The second term in Eq. (11) can be further simplified by transforming Γ into a diagonal form via its singular value decomposition [29]. More precisely, exploiting the fact that Γ is real we can express it as

$$\Gamma = O^T \begin{bmatrix} \gamma_1 & 0 & 0 \\ 0 & \gamma_2 & 0 \\ 0 & 0 & \gamma_3 \end{bmatrix} \Omega, \quad (12)$$

where O and Ω are real orthogonal matrices of $\text{SO}(3)$ while $\{\gamma_i\}$ are real (not necessarily non-negative) quantities whose moduli correspond to the singular eigenvalues of Γ [30]. We can then define the two set of vectors

$$\hat{w}_k = \sum_{j=1}^3 O_{kj} \hat{x}_j, \quad \hat{v}_k = \sum_{j=1}^3 \Omega_{kj} \hat{x}_j \quad (13)$$

for $k = 1, 2, 3$. As $O, \Omega \in \text{SO}(3)$, by construction $\{\hat{w}_k\}$ is an orthonormal (right-hand oriented) set of real vectors and so is $\{\hat{v}_k\}$ (each is indeed a rotation of the Cartesian unit vectors $\{\hat{x}_j\}$). Using the above, we can arrange Eq. (11) as

$$M(\hat{e}) = (\vec{x}_{A\perp} \cdot \vec{\sigma}_A) \otimes \mathbb{1}_B + \sum_{k=1}^3 \gamma_k (\vec{w}_{k\perp} \cdot \vec{\sigma}_A) \otimes (\hat{v}_k \cdot \vec{\sigma}_B), \quad (14)$$

where for compactness of notation we introduced the vectors

$$\vec{x}_{A\perp} = \vec{x}_A - (\hat{e} \cdot \vec{x}_A)\hat{e}, \quad \vec{w}_{k\perp} = \hat{w}_k - (\hat{e} \cdot \hat{w}_k)\hat{e} \quad (15)$$

to represent the orthogonal component of \vec{x}_A and \hat{w}_k with respect to \hat{e} .

Note that $\{\hat{v}_k \cdot \vec{\sigma}_B\}$ describes the transformed set of Pauli matrices under a local rotation on B . This set clearly fulfills all the properties of Pauli matrices as well. One can therefore redefine the B 's Pauli matrices as $\{\hat{v}_k \cdot \vec{\sigma}_B\} \rightarrow \sigma_{Bk}$, which amounts to applying a local unitary on B . Let then $M'(\hat{e})$ be the transformed operator obtained from $M(\hat{e})$ under such rotation, i.e.

$$M'(\hat{e}) = (\vec{x}_{A\perp} \cdot \vec{\sigma}_A) \otimes \mathbb{1}_B + \sum_{k=1}^3 \gamma_k (\vec{w}_{k\perp} \cdot \vec{\sigma}_A) \otimes \sigma_{Bk}. \quad (16)$$

Since the trace norm is invariant under any local unitary we have

$$\|M(\hat{e})\|_1 = \|M'(\hat{e})\|_1 \quad (17)$$

in line with the invariance property *ii*) of $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$ [indeed $M'(\hat{e})$ is the operator (11) associated to the state ρ'_{AB} obtained from ρ_{AB} via a local unitary rotation associated to the transformation $\{\hat{v}_k \cdot \vec{\sigma}_B\} \rightarrow \sigma_{Bk}$]. The trace norm of $M'(\hat{e})$ can now be computed by diagonalizing the operator $M'(\hat{e})^\dagger M'(\hat{e})$. For this purpose, we recall that given two arbitrary vectors $\{\vec{x}, \vec{y}\}$, the Pauli matrices fulfill the following commutation and anti-commutation relations

$$[\vec{x} \cdot \vec{\sigma}_A, \vec{y} \cdot \vec{\sigma}_A] = 2i(\vec{x} \wedge \vec{y}) \cdot \vec{\sigma}_A, \quad (18)$$

$$\{\vec{x} \cdot \vec{\sigma}_A, \vec{y} \cdot \vec{\sigma}_A\} = 2(\vec{x} \cdot \vec{y}) \quad (19)$$

as well as the identities $\sigma_{A1}\sigma_{A2} = i\sigma_{A3}$, $\sigma_{A2}\sigma_{A1} = -i\sigma_{A3}$ and the analogous identities obtained through cyclic permutations (in the above expression “ \wedge ” indicates the **cross** product). Using these, we straightforwardly end up with

$$M'(\hat{e})^\dagger M'(\hat{e}) = (Q + x_{A\perp}^2) \mathbb{1}_{AB} + \Delta + 2 \mathbb{1}_A \otimes \vec{\chi} \cdot \vec{\sigma}_B, \quad (20)$$

where $x_{A\perp} = |\vec{x}_{A\perp}|$ (throughout, $x = |\vec{x}|$ for any vector \vec{x}), $\vec{\chi}$ is a tridimensional real vector of components

$$\chi_k = \gamma_k \vec{w}_{k\perp} \cdot \vec{x}_{A\perp}, \quad (21)$$

while Q is a positive quantity defined as

$$Q = \sum_{k=1}^3 \gamma_k^2 |\vec{w}_{k\perp}|^2, \quad (22)$$

and finally Δ is the operator

$$\begin{aligned} \Delta &= \sum_{j \neq k} \gamma_j \gamma_k [(\vec{w}_{j\perp} \cdot \vec{\sigma}_A)(\vec{w}_{k\perp} \cdot \vec{\sigma}_A) \otimes \sigma_{Bj} \sigma_{Bk}] \\ &= -2\gamma_1 \gamma_2 (\vec{w}_{1\perp} \wedge \vec{w}_{2\perp}) \cdot \vec{\sigma}_A \otimes \sigma_{B3} \\ &\quad -2\gamma_2 \gamma_3 (\vec{w}_{2\perp} \wedge \vec{w}_{3\perp}) \cdot \vec{\sigma}_A \otimes \sigma_{B1} \\ &\quad -2\gamma_3 \gamma_1 (\vec{w}_{3\perp} \wedge \vec{w}_{1\perp}) \cdot \vec{\sigma}_A \otimes \sigma_{B2}. \end{aligned} \quad (23)$$

This expression can be simplified by observing that since the $\vec{w}_{k\perp}$'s are vectors orthogonal to \hat{e} [see Eq. (15)] their mutual **cross** products must be collinear with the latter. Indeed, introducing the spherical coordinates $\{\theta, \phi\}$ which specify \hat{e} in the reference frame defined by $\{\hat{w}_k\}$, we have

$$\begin{aligned}(\vec{w}_{1\perp} \wedge \vec{w}_{2\perp}) &= (\hat{w}_3 \cdot \hat{e}) \hat{e} = \cos \theta \hat{e}, \\(\vec{w}_{2\perp} \wedge \vec{w}_{3\perp}) &= (\hat{w}_1 \cdot \hat{e}) \hat{e} = \sin \theta \cos \phi \hat{e}, \\(\vec{w}_{3\perp} \wedge \vec{w}_{1\perp}) &= (\hat{w}_2 \cdot \hat{e}) \hat{e} = \sin \theta \sin \phi \hat{e}.\end{aligned}\quad (24)$$

Substituting these identities in Eq. (23), the operator Δ can remarkably be arranged in terms of a simple tensor product as

$$\Delta = -2(\hat{e} \cdot \vec{\sigma}_A) \otimes (\vec{g} \cdot \vec{\sigma}_B), \quad (25)$$

where \vec{g} is the vector

$$\vec{g} = (\gamma_2 \gamma_3 \sin \theta \cos \phi, \gamma_3 \gamma_1 \sin \theta \sin \phi, \gamma_1 \gamma_2 \cos \theta), \quad (26)$$

which is orthogonal to $\vec{\chi}$ [31]. Next, observe that the operator $\hat{e} \cdot \vec{\sigma}_A$ of Eq. (25) is Hermitian with eigenvalues 1 and -1 . Therefore, if $\{|0\rangle_A, |1\rangle_A\}$ are its eigenvectors we can write $\hat{e} \cdot \vec{\sigma}_A = |0\rangle_A \langle 0| - |1\rangle_A \langle 1|$. Plugging this and $\mathbb{1}_A = |0\rangle_A \langle 0| + |1\rangle_A \langle 1|$ into Eq. (20) this can be arranged as

$$\begin{aligned}M'(\hat{e})^\dagger M'(\hat{e}) &= (Q + x_{A\perp}^2) \mathbb{1}_{AB} \\&+ 2[|0\rangle_A \langle 0| \otimes (\vec{\chi} - \vec{g}) \cdot \vec{\sigma}_B + |1\rangle_A \langle 1| \otimes (\vec{\chi} + \vec{g}) \cdot \vec{\sigma}_B],\end{aligned}$$

which can now be put in diagonal form. Indeed, due to the aforementioned spectrum of $\vec{\chi} \cdot \vec{\sigma}$, it has eigenvalues $\lambda = Q + x_{A\perp}^2 \pm 2\sqrt{\chi^2 + g^2}$, each twofold degenerate [31]. Therefore, through Eq. (17) we end up with

$$\|M(\hat{e})\|_1 = 2 \left(\sqrt{a + \sqrt{b}} + \sqrt{a - \sqrt{b}} \right), \quad (27)$$

where

$$a = a(\hat{e}) = Q + x_{A\perp}^2 = Q + x_A^2 - (\vec{\chi}_A \cdot \hat{e})^2, \quad (28)$$

$$b = b(\hat{e}) = 4(\chi^2 + g^2). \quad (29)$$

Note that Q , $x_{A\perp}$, χ and g are all functions of \hat{e} [cf. Eqs. (21), (22) and (26)]. As $\|M(\hat{e})\|_1$ is a positive-definite function, finding its minimum is equivalent to searching for the minimum of its square $\|M(\hat{e})\|_1^2$. Thereby

$$\min_{\hat{e}} \|M(\hat{e})\|_1 = \sqrt{\min_{\hat{e}} \|M(\hat{e})\|_1^2} = 2 \sqrt{2 \left[\min_{\hat{e}} h(\hat{e}) \right]}, \quad (30)$$

where the function $h(\hat{e})$ is defined as

$$h(\hat{e}) = a(\hat{e}) + \sqrt{a^2(\hat{e}) - b(\hat{e})}. \quad (31)$$

In conclusion, in the light of Eqs. (10), (27) and (30)

$$\begin{aligned}\mathcal{D}^{(\rightarrow)}(\rho_{AB}) &= \frac{1}{4} \min_{\hat{e}} \left[\sqrt{a + \sqrt{b}} + \sqrt{a - \sqrt{b}} \right] \\&= \frac{1}{4} \sqrt{2 \left[\min_{\hat{e}} h \right]}.\end{aligned}\quad (32)$$

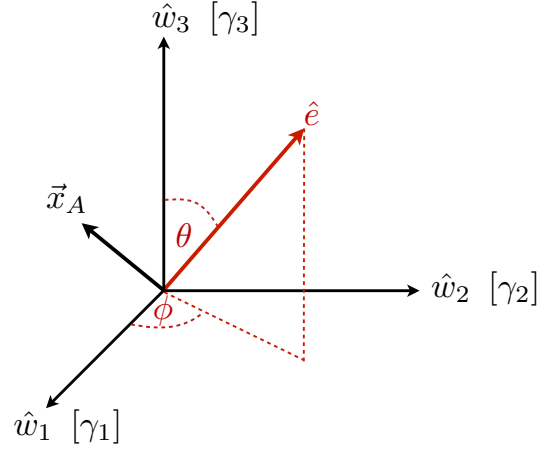


FIG. 1: (Color online) Schematics of the minimization procedure for calculating the trace distance discord $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$ of a two-qubit state ρ_{AB} . The reference frame in which this is carried out is defined by the orthonormal set of three vectors $\{\hat{w}_k\}$, where each \hat{w}_k is associated with a real singular eigenvalue γ_k of the correlation matrix [see Eqs. (8), (12) and (13)]. This frame identifies a representation for the local Bloch vector \vec{x}_A [defined in Eq. (7)]. All these quantities are drawn using solid black lines to highlight that, for a given density matrix ρ_{AB} , they are fixed. Instead, the unit vector \hat{e} (red line) represents the direction along which a projective measurement on A is performed. In the optimization procedure, \hat{e} is varied until function h in Eq. (31) reaches its global minimum according to Eq. (32).

We have thus expressed our trace-norm-based measure of QCs of an arbitrary state ρ_{AB} as the minimum of an *explicit* function of the two angles $\{\theta, \phi\}$ ($0 \leq \theta \leq \pi$, $0 \leq \phi \leq 2\pi$). Equation (32) is the first main finding of this paper. For clarity, all quantities involved in the minimization problem under investigation are pictorially represented in Fig. 1.

III. BELL DIAGONAL STATES AND STATES WITH HOMOGENEOUS SINGULAR VALUES

The optimization in Eq. (32) simplifies when the state possesses certain symmetries. In particular, by ordering the singular eigenvalues of Γ as (this convention is adopted only in the present section)

$$|\gamma_1| \geq |\gamma_2| \geq |\gamma_3|, \quad (33)$$

one can show that

$$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{|\gamma_2|}{2}, \quad (34)$$

at least for two classes of states ρ_{AB} , which we label as ‘A’ and ‘B’, respectively. These are defined as

class A : arbitrary $\{\gamma_k\}$ but $\vec{x}_A = 0$

class B : arbitrary \vec{x}_A but $\{\gamma_k\}$ with the equal moduli, i.e.

$$|\gamma_k| = \gamma \quad \forall k = 1, 2, 3. \quad (35)$$

We develop the proof in the following two subsections.

A. Bell diagonal states

States of class A, which include Bell diagonal states, are characterized by the property that the reduced density matrix of subsystem A is maximally mixed. For these, Eq. (32) was proven in Refs. [12, 13] using an independent approach. Here, we present an alternative (possibly simpler) derivation based on Eq. (32). We point out that these states form a special subset of X states, which we will study in full detail in Section V. Here, our goal is indeed to present a straightforward application of our method for calculating the TDD developed in the previous Section.

To begin with, we observe that if $\vec{x}_A = 0$ then the vector $\vec{\chi}$ in Eq. (21) vanishes, i.e. $\vec{\chi} = 0$, while the function a in Eq. (28) coincides with Q in Eq. (22). Thereby, the function h in Eq. (31), which we have to minimize over \hat{e} according to Eq. (32), becomes

$$h = Q + \sqrt{H} \quad \text{with} \quad H = Q^2 - 4g^2. \quad (36)$$

Expressing now Q in terms of θ and ϕ and due to the ordering in Eq. (33), it turns out that

$$Q(\theta, \phi) = \gamma_1^2(1 - \cos^2 \phi \sin^2 \theta) + \gamma_2^2(1 - \sin^2 \phi \sin^2 \theta) + \gamma_3^2(1 - \cos^2 \theta) \geq Q(\theta = \pi/2, \phi = 0) = \gamma_2^2 + \gamma_3^2, \quad (37)$$

namely Q reaches its minimum value for $\theta = \pi/2$ and $\phi = 0$, i.e. when \hat{e} points toward \hat{w}_1 . The same property holds for the function H . Indeed one has

$$H(\theta, \phi) = A(\theta) \sin^4 \phi + B(\theta) \sin^2 \phi + C(\theta) \geq H(\theta = \pi/2, \phi = 0) = (\gamma_2^2 - \gamma_3^2)^2, \quad (38)$$

where we used

$$\begin{aligned} A(\theta) &= \sin^4 \theta (\gamma_1^2 - \gamma_2^2)^2 \geq A(0) = 0, \\ B(\theta) &= 2 \sin^2 \theta (\gamma_1^2 - \gamma_2^2)(\gamma_2^2 - \gamma_3^2) \\ &\quad + \cos^2 \theta (\gamma_1^2 - \gamma_3^2) \geq B(0) = 0, \\ C(\theta) &= (\gamma_2^2 - \gamma_3^2)^2 + 2 \cos^2 \theta (\gamma_2^2 + \gamma_3^2) (\gamma_1^2 - \gamma_3^2) \\ &\quad + \cos^4 \theta (\gamma_1^2 - \gamma_3^2)^2 \geq C(\theta = \pi/2) \geq (\gamma_2^2 - \gamma_3^2)^2. \end{aligned}$$

Replacing Eq. (37) and (38) into Eq. (36) entails $h(\theta, \phi) \geq h(\theta = \pi/2, \phi = 0) \geq 2|\gamma_2|$, which through Eq. (32) yields Eq. (34).

B. States with homogeneous $|\gamma_k|$'s

Class B (see definition given above) includes, for instance, mixtures of the form $\rho_{AB} = p\rho_A \otimes \mathbb{1}_B/2 + (1-p)|\Psi_-\rangle_{AB}\langle\Psi_-|$ where $p \in [0, 1]$, ρ_A is an arbitrary state of A , and $|\Psi_-\rangle$ is the singlet state $|\Psi_-\rangle = (|01\rangle_{AB} - |10\rangle_{AB})/\sqrt{2}$ [from now on, $\{|0\rangle_{A(B)}, |1\rangle_{A(B)}\}$ denotes an orthonormal basis for A (B)]. In this case, $\gamma_k = (1-p)$ for all k while $\vec{x}_A = p\vec{s}_A$ with \vec{s}_A the Bloch vector of ρ_A : therefore according to Eq. (34) this state has a value for TDD given by $(1-p)/2$.

To derive Eq. (34), we introduce the diagonal matrix $T = \text{diag}(t_{11}, t_{22}, t_{33})$ formed by the coefficients t_{11}, t_{22}, t_{33} defined by the identities

$$\gamma_j = t_{jj} \gamma, \quad (39)$$

[it is clear from (35) that t_{jj} can only take values ± 1]. Under this condition, from Eqs. (21), (22) and (26) it then follows

$$\begin{aligned} Q &= 2\gamma^2 \\ \vec{g} &= \xi \gamma^2 T \hat{e} \implies |\vec{g}|^2 = \gamma^4, \\ \vec{\chi} &= \gamma T \vec{x}_{A,\perp} \implies |\vec{\chi}|^2 = \gamma^2 |\vec{x}_{A,\perp}|^2, \end{aligned} \quad (40)$$

where ξ takes value either 1 or -1 depending on the explicit form of the mapping (39). Replacing this into Eqs. (28), (29) and (31) we end up with

$$h = 2\gamma^2 + 2|\vec{x}_{A,\perp}|^2, \quad (41)$$

which depends upon \hat{e} through $|\vec{x}_{A,\perp}|^2$ only. The minimum is then achieved when $|\vec{x}_{A,\perp}|$ vanishes, which clearly occurs by taking \hat{e} along the direction of \vec{x}_A [recall Eq. (15)]. Thus

$$\min_{\hat{e}} h = 2\gamma^2 \quad (42)$$

which when replaced into Eq. (32) gives Eq. (34), as anticipated.

IV. CORRELATION MATRIX WITH A SINGLE NON-ZERO SINGULAR EIGENVALUE

This class of states is important since quantum-classical states fall within it, as we show later. It is defined by [see Eq. (12)] $\gamma_2 = \gamma_3 = 0$ while $\gamma_1 = \gamma$ and \vec{x}_A are arbitrary (the only constraint is that the resulting ρ_{AB} must be a properly defined density matrix). We show below that the TDD of one such state is given by

$$\mathcal{D}^{(\leftrightarrow)}(\rho_{AB}) = \frac{|\vec{\gamma}_1 \wedge \vec{x}_A|}{2} \min \left\{ \frac{1}{|\vec{\gamma}_1 \pm \vec{x}_A|} \right\}, \quad (43)$$

where $\vec{\gamma}_1 = |\gamma_1| \hat{w}_1$, \hat{w}_1 being the first element of the set $\{\hat{w}_k\}$ defined in Eq. (13). Eq. (43) is another main finding of this work.

To begin with, we observe that due to $\gamma_2 = \gamma_3 = 0$ we are free to choose the direction of the Cartesian axes \hat{w}_2 and \hat{w}_3 ($\hat{w}_2 \perp \hat{w}_3$) on the plane orthogonal to \hat{w}_1 . We thus take \hat{w}_2 as lying on the plane formed by \hat{w}_1 and \vec{x}_A . Hence we can write $\vec{x}_A = \tilde{x}_{A1} \hat{w}_1 + \tilde{x}_{A2} \hat{w}_2$, where \tilde{x}_{A1} and \tilde{x}_{A2} are the components of \vec{x}_A in reference frame defined by $\{\hat{w}_k\}$. Accordingly,

$$\tilde{x}_{A1} = \hat{x}_A \cdot \hat{w}_1 = x_A \cos \alpha, \quad \tilde{x}_{A2} = \hat{x}_A \cdot \hat{w}_2 = x_A \sin \alpha \quad (44)$$

with α being the angle between \vec{x}_A and \hat{w}_1 while $x_A = \sqrt{\tilde{x}_{A1}^2 + \tilde{x}_{A2}^2}$. With the help of Eqs. (21), (22) and (26), in the present case a and b [cf. Eqs. (28) and (29)] read

$$a = \gamma^2 + x_A^2 - [\gamma^2 \tilde{e}_1^2 + (\tilde{e} \cdot \vec{x}_A)^2], \quad b = 4\gamma^2 [\tilde{x}_{A1} - \tilde{e}_1(\tilde{e} \cdot \vec{x}_A)]^2, \quad (45)$$

where $\tilde{e}_1 = \hat{e} \cdot \hat{w}_1$. Observe then that we can write

$$a \pm \sqrt{b} = (\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2 - [\gamma \tilde{e}_1 \pm (\hat{e} \cdot \tilde{x}_A)]^2. \quad (46)$$

It turns out that *both* $a + \sqrt{b}$ and $a - \sqrt{b}$ decrease when the component of \hat{e} on the plane formed by \hat{w}_1 and \tilde{x}_A , i.e., the $\hat{w}_1 - \hat{w}_2$ plane, grows. To see this, we decompose \hat{e} as $\hat{e} = \vec{e} + \vec{e}_\perp$, where $\vec{e} = \tilde{e}_1 \hat{w}_1 + \tilde{e}_2 \hat{w}_2$ is the component of \hat{e} on the $\hat{w}_1 - \hat{w}_2$ plane, while $\vec{e}_\perp = \tilde{e}_3 \hat{w}_3$ the one orthogonal to it. With these definitions, in Eq. (46) we can evidently replace \hat{e} with \vec{e} (we remind that $\tilde{x}_{A3} = 0$). Now, it should be evident that the last term of Eq. (46) can be written as $-[\gamma \tilde{e}_1 \pm (\hat{e} \cdot \tilde{x}_A)]^2 = -|\vec{e}|^2 [f_\pm(\phi, \alpha)]^2$, where $f_\pm(\phi, \alpha) = \gamma \cos \phi \pm x_A \cos(\phi - \alpha)$ is a function of ϕ (i.e., the azimuthal angle of \hat{e}) and the aforementioned α . Clearly, for given ϕ the minimum of $a \pm \sqrt{b}$ is achieved when $|\vec{e}|$ is maximum, i.e., for $\vec{e} \equiv \hat{e}$ or equivalently $\theta = \pi/2$. Thus, due to Eq. (27), in Eq. (32) we can safely restrict the minimization over $\hat{e} = (\theta, \phi)$ to the set $\hat{e} = (\pi/2, \phi)$. To summarize, we need to calculate

$$\min_{\phi} \left[\|M(\hat{e})\|_1 \right]_{\theta=\pi/2} = 2 \sum_{\eta=\pm} \sqrt{(\gamma + \eta \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2 - f_\eta(\phi, \alpha)^2}. \quad (47)$$

Through few straightforward steps (see Appendix A), $\|M(\hat{e})\|_1$ can be arranged as (we henceforth omit to specify $\theta = \pi/2$)

$$\|M(\hat{e})\|_1 = 2 \sum_{\eta=\pm} |x_A \sin(\phi - \alpha) + \eta \gamma \sin \phi|. \quad (48)$$

Exploiting the positiveness of $\|M(\hat{e})\|_1$ and the identity $(|y+z| + |y-z|)^2 = 4 \max\{y^2, z^2\}$, where y and z are any two real numbers, Eq. (48) can be converted into

$$\begin{aligned} \|M(\hat{e})\|_1 &= 4 \max\{|x_A \sin(\phi - \alpha)|, |\gamma \sin \phi|\} \\ &= 4 \sqrt{x_A^2 + \gamma^2} \max\{|\sin \beta \sin(\phi - \alpha)|, |\cos \beta \sin \phi|\}, \end{aligned} \quad (49)$$

where the angle β is defined through the identity

$$\sin \beta = |x_A| / \sqrt{x_A^2 + \gamma^2}. \quad (50)$$

Replacing $\|M(\hat{e})\|$ so obtained into Eq. (10) we can then express the one-sided TDD of our state ρ_{AB} in terms of the following min-max problem,

$$\begin{aligned} \mathcal{D}^{(\rightarrow)}(\rho_{AB}) &= \frac{\sqrt{x_A^2 + \gamma^2}}{2} \\ &\times \min_{\phi \in [0, 2\pi]} \max\{|\sin \beta \sin(\phi - \alpha)|, |\cos \beta \sin \phi|\}. \end{aligned} \quad (51)$$

An analytic solution is obtained by observing that the ϕ -dependent functions $f_1(\phi) = |\sin \beta \sin(\phi - \alpha)|$ and $f_2(\phi) = |\cos \beta \sin \phi|$ have the same period π and that in the domain $\phi \in [0, \pi]$ exhibit the two crossing points ϕ_{c+} and ϕ_{c-} given by

$$\cot(\phi_{c\pm}) = \cot \alpha \pm \left| \frac{\cot \beta}{\sin \alpha} \right|. \quad (52)$$

By construction, the function Eq. (49) reaches its minimum either in ϕ_{c+} or in ϕ_{c-} . Therefore,

$$\begin{aligned} \mathcal{D}^{(\rightarrow)}(\rho_{AB}) &= \frac{\sqrt{x_A^2 + \gamma^2}}{2} \min\{|\cos \beta \sin(\phi_{c+})|, |\cos \beta \sin(\phi_{c-})|\} \\ &= \frac{|\gamma \tilde{x}_{A2}|}{2} \min \left\{ \frac{1}{\sqrt{(\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2}} \right\}, \end{aligned} \quad (53)$$

where the latter identity have been obtained through simple algebraic manipulations. To arrange this formula in a form independent of the reference frame, we make use of Eqs. (44) and (50). This finally yields Eq. (43).

A. Quantum-classical states

The result of the previous section can be exploited to provide an analytical closed formula of $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$ for the well-known class of quantum-classical states. One such state reads

$$\rho_{AB} = p \rho_{0A} \otimes |0\rangle_B \langle 0| + (1-p) \rho_{1A} \otimes |1\rangle_B \langle 1|, \quad (54)$$

where $\rho_{0(1)}$ is an arbitrary single-qubit state with associated Bloch vector $\vec{s}_{0(1)}$, i.e., $\rho_{0(1)} = (\mathbb{1} + \vec{s}_{0(1)} \cdot \vec{\sigma})/2$. The state in Eq. (54) represents a paradigmatic example of a separable state which is still able to feature $A \rightarrow B$ quantum correlations. On the other hand, note that the quantum discord in the opposite direction, $B \rightarrow A$, is zero by construction.

One can assume without loss of generality that $\vec{s}_0 = (0, 0, s_0)$ and $\vec{s}_1 = (s_1 \sin \varphi, 0, s_1 \cos \varphi)$ with $0 \leq \varphi \leq \pi$, i.e., the Z-axis of the Bloch sphere is taken along the direction of \vec{s}_0 while the Y-axis lies orthogonal to the plane containing both \vec{s}_0 and \vec{s}_1 . Vector \tilde{x}_A and matrix Γ are calculated as

$$\tilde{x}_A = ((1-p)s_1 \sin \varphi, 0, ps_0 + (1-p)s_1 \cos \varphi), \quad (55)$$

$$\Gamma = \begin{pmatrix} 0 & 0 & (p-1)s_1 \sin \varphi \\ 0 & 0 & 0 \\ 0 & 0 & ps_0 + (1-p)s_1 \cos \varphi \end{pmatrix}. \quad (56)$$

Γ has only one singular eigenvalue since its singular value decomposition yields $\gamma_2 = \gamma_3 = 0$ and

$$|\gamma_1| = \gamma = \sqrt{p^2 s_0^2 + (p-1)s_1 [(p-1)s_1 + 2ps_0 \cos \varphi]}. \quad (57)$$

Such states therefore fall exactly in the case studied in the previous section. To apply Eq. (43), though, we need to calculate the unit vectors \hat{w}_k . From the matrix Eq. (56), they are calculated as

$$\hat{w}_1 = \frac{1}{\Delta_1} ((p-1)s_1 \sin \varphi, 0, ps_0 + (p-1)s_1 \cos \varphi), \quad (58)$$

$$\hat{w}_2 = \frac{1}{\Delta_2} \left(\frac{(1-p)s_1 \cot \varphi - ps_0 \csc \varphi}{(p-1)s_1}, 0, 1 \right), \quad (59)$$

$$\hat{w}_3 = (0, 1, 0), \quad (60)$$

where $\Delta_{1,2}$ are normalization coefficients. In particular, it turns that Δ_1 coincides with γ in Eq. (57), i.e. $\Delta_1 = \gamma$. Hence, the vector $\vec{\gamma}_1 = \gamma \hat{w}_1$ in Eq. (43) is given by

$$\vec{\gamma}_1 = ((p-1)s_1 \sin \varphi, 0, ps_0 + (p-1)s_1 \cos \varphi). \quad (61)$$

This, together with Eq. (55), yields the identities

$$\begin{aligned} |\tilde{x}_A \wedge \vec{\gamma}_1| &= 2p(1-p)s_0 s_1 |\sin \varphi|, \\ |\vec{\gamma}_1 + \tilde{x}_A| &= 2p s_0, \\ |\vec{\gamma}_1 - \tilde{x}_A| &= 2(1-p)s_1. \end{aligned}$$

Replacing these into Eq. (43), we end up with

$$\mathcal{D}^{(\leftrightarrow)}(\rho_{AB}) = \frac{|\sin \varphi|}{2} \min\{ps_0, (1-p)s_1\}, \quad (62)$$

which represents the TDD of the most general quantum-classical state [Eq. (54)]. This has a very clear interpretation once one notices that the maximum value of $\mathcal{D}^{(\leftrightarrow)}$ is 1/4 and is taken for $s_0 = s_1 = 1$, $p = 1/2$ and $\varphi = \pi/2$. For these parameters, Eq. (54) reduces to $\rho_{AB} = 1/2(|0\rangle_A\langle 0| \otimes |0\rangle_B\langle 0| + |+\rangle_A\langle +| \otimes |1\rangle_B\langle 1|)$ (where $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$), which is a popular instance of separable quantum-correlated state. The qualitative behavior of \mathcal{D} for $s_0 = s_1$ and $p = 1/2$ is fully in line with that of the quantum discord [25] and for $s_0 = s_1 = 1$ with that of the fidelity-based measure analyzed in Ref. [24].

V. X STATES

A two-qubit X state has the X -shaped matrix form

$$\rho_{AB} = \begin{pmatrix} \rho_{11} & 0 & 0 & \rho_{41}^* \\ 0 & \rho_{22} & \rho_{32}^* & 0 \\ 0 & \rho_{32} & \rho_{33} & 0 \\ \rho_{41} & 0 & 0 & \rho_{44} \end{pmatrix} \quad (63)$$

$$\begin{aligned} & \text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 < 0 & \mathcal{D}^{(\leftrightarrow)}(\rho_{AB}) &= \frac{|\gamma_1|}{2}, \\ & \text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geq 0 & \begin{cases} \text{if } |\gamma_3| \geq |\gamma_1| & \mathcal{D}^{(\leftrightarrow)}(\rho_{AB}) = \frac{|\gamma_1|}{2} \\ \text{if } |\gamma_3| < |\gamma_1| & \mathcal{D}^{(\leftrightarrow)}(\rho_{AB}) = \Theta\left(\gamma_1^2 - \gamma_3^2 + x_{A3}^2\right)^{\frac{1}{2}} \sqrt{\frac{\gamma_1^2(\gamma_3^2 + x_{A3}^2) - \gamma_2^2\gamma_3^2}{\gamma_1^2 - \gamma_3^2 + x_{A3}^2}} + \Theta\left[-\left(\gamma_1^2 - \gamma_3^2 + x_{A3}^2\right)\right] \frac{|\gamma_3|}{2}, \end{cases} \end{aligned} \quad (65)$$

where we have used the Heaviside step function $\Theta(x)$ [we adopt the standard convention $\Theta(0) = 1/2$]. It can be checked (see Appendix B) that for Bell-diagonal states the above expression reproduces the result of Section III, i.e., the TDD is half the intermediate value among $\{|\gamma_k|\}$ [we stress that here the labelling of the γ_k 's does not imply the ordering in Eq. (33)].

Equation (65) can also be written in the compact form

$$\mathcal{D}^{(\leftrightarrow)}(\rho_{AB}) = \frac{1}{2} \sqrt{\frac{\gamma_1^2 \max\{\gamma_3^2, \gamma_2^2 + x_{A3}^2\} - \gamma_2^2 \min\{\gamma_3^2, \gamma_1^2\}}{\max\{\gamma_3^2, \gamma_2^2 + x_{A3}^2\} - \min\{\gamma_3^2, \gamma_1^2\} + \gamma_1^2 - \gamma_2^2}}, \quad (66)$$

showing that for the X -states the discord is only a function of the following three parameters: $|\gamma_1|$, $|\gamma_3|$ and $\sqrt{\gamma_2^2 + x_{A3}^2}$.

To begin with, Eqs. (28) and (29) imply that the (θ, ϕ) -dependent functions a and b entering Eq. (31) [recall that (θ, ϕ) specify \hat{e}] depend only on $\mu \equiv \sin^2 \theta$ and $\nu \equiv \sin^2 \phi$ as

$$a = a_0 + a_1 \mu, \quad b = b_0 + b_1 \mu + b_2 \mu^2, \quad (67)$$

subject to the constraints $\sum_{i=1}^4 \rho_{ii} = 1$, $\rho_{11}\rho_{44} \geq |\rho_{14}|^2$ and $\rho_{22}\rho_{33} \geq |\rho_{23}|^2$. Here, we have referred to the computational basis $\{|00\rangle_{AB}, |01\rangle_{AB}, |10\rangle_{AB}, |11\rangle_{AB}\}$. Without loss of generality, off-diagonal entries ρ_{32} and ρ_{41} can be taken as positive, i.e., $\rho_{32} \geq 0$ and $\rho_{41} \geq 0$ [32]. It is straightforward to check that for such states $x_{A,1} = x_{A,2} = 0$, $x_{A3} = 2(\rho_{11} + \rho_{22}) - 1$ (that is, \vec{x}_A lies along the \hat{x}_3 -axis) while the correlation matrix has already the diagonal form since $\Gamma = \text{diag}\{\gamma_1, \gamma_2, \gamma_3\}$ with

$$\gamma_1 = 2(\rho_{32} + \rho_{41}), \quad \gamma_2 = 2(\rho_{32} - \rho_{41}), \quad \gamma_3 = 1 - 2(\rho_{22} + \rho_{33}). \quad (64)$$

Hence, in the present case $\hat{w}_k = \hat{x}_k$ for $k = 1, 2, 3$ [see Eq. (13)]. We therefore have to deal with the four parameters x_{A3} and $\{\gamma_k\}$. Note that the only hierarchical relation which always holds is $|\gamma_1| \geq |\gamma_2|$ [see Eq. (64)].

In what follows, we will prove that the TDD of state Eq. (63) is given by

where $\{a_i\}$ and $\{b_i\}$ are the following linear functions of ν

$$a_0 = \gamma_1^2 + \gamma_2^2, \quad a_1 = (\gamma_3^2 + x_{A3}^2 - \gamma_1^2) + (\gamma_1^2 - \gamma_2^2)\nu, \quad (68)$$

$$b_0 = 4\gamma_1^2\gamma_2^2, \quad b_2 = 4x_{A3}^2[(\gamma_3^2 - \gamma_1^2) + (\gamma_1^2 - \gamma_2^2)\nu], \quad (69)$$

$$b_1 = 4[\gamma_2^2\gamma_3^2 + \gamma_1^2(x_{A3}^2 - \gamma_2^2) + (\gamma_1^2 - \gamma_2^2)(\gamma_3^2 - x_{A3}^2)\nu]. \quad (70)$$

Clearly, $a(\mu, \nu)$ and $b(\mu, \nu)$ are defined in the square \mathcal{S} defined by $\mathcal{S} \equiv \{\mu, \nu: 0 \leq \mu \leq 1, 0 \leq \nu \leq 1\}$ [and so is $h = a + \sqrt{a^2 - b}$, see Eq. (31)]. The partial derivative of h with respect to ν , $\partial_\nu h$, can be arranged as $\partial_\nu h = (2h\partial_\nu a - \partial_\nu b) / (2\sqrt{a^2 - b})$ (an analogous formula holds for $\partial_\mu h$). Now, due to Eqs. (67)-(70) $\partial_\nu a = (\gamma_1^2 - \gamma_2^2)\mu$ and, notably, $\partial_\nu b = 4[\gamma_3^2 + (\mu - 1)x_{A3}^2]\partial_\nu a$. When these are replaced in $\partial_\nu h$ we thus end up with

$$\partial_\nu h = \frac{h - 2[\gamma_3^2 + x_{A3}^2(\mu - 1)]}{\sqrt{a^2 - b}} \partial_\nu a. \quad (71)$$

As witnessed by the denominator of this equation, we observe that function h is in general non-differentiable at points such that $a^2 = b$, owing to the square root $\sqrt{a^2 - b}$ appearing in its

definition, Eq. (31). One then has to investigate these points carefully, as they may potentially yield extremal values of h that would not be found by simply imposing $\partial_\mu h = \partial_\nu h = 0$.

As a key step in our reasoning, we first demonstrate that a minimum of h cannot occur in the interior of \mathcal{S} . Afterward, we minimize function h on the boundary of \mathcal{S} , which will eventually lead to formula (65).

A. Proof that minimum points cannot lie in the interior of \mathcal{S}

We first address minimum points at which h is differentiable, i.e., that fulfill $a^2 \neq b$ entailing the existence of partial derivatives for h . A necessary condition for h to take a minimum on these points is then $\partial_\nu h = 0$. Based on Eq. (71), this can happen when either $h = h_0 = 2[\gamma_3^2 + x_{A3}^2(\mu - 1)]$ or $\partial_\nu a = 0$.

In the latter case, as discussed above, $\partial_\nu a = (\gamma_1^2 - \gamma_2^2)\mu$, which vanishes for $\mu = 0$ (that is on the boundary of \mathcal{S}) or $|\gamma_1| = |\gamma_2|$. Using Eq. (31) and Eqs. (67) through (70) it is easy to calculate that when $|\gamma_1| = |\gamma_2|$, depending on the sign of $\gamma_2^2 - \gamma_3^2 + x_{A3}^2$, either $h = 2(\gamma_2^2 + x_{A3}^2\mu)$ or $h = 2[\gamma_2^2 + (\gamma_3^2 - \gamma_2^2)\mu]$. Thereby, in the case $|\gamma_1| = |\gamma_2|$ the minima of h must fall on the boundary of \mathcal{S} .

Let us now analyze the situation where $h = h_0 = 2[\gamma_3^2 + x_{A3}^2(\mu - 1)]$, which would also yield $\partial_\nu h = 0$ [cf. Eq. (71)]. As $h = a + \sqrt{a^2 - b}$, a necessary condition for this to occur is clearly $(h_0 - a)^2 = a^2 - b$. With the help of Eqs. (67)-(70), this identity can be explicitly written as $4(1-\mu)(\gamma_1^2 - \gamma_3^2 + x_{A3}^2)(\gamma_2^2 - \gamma_3^2 + x_{A3}^2) = 0$. This is fulfilled if at least one of the following identities holds: (i) $\mu = 1$, (ii) $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 = 0$, (iii) $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 = 0$. Case (i) clearly corresponds to a point on the boundary of \mathcal{S} . In case (ii), using that $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 \leq 0$ (due to $\gamma_2^2 \leq \gamma_1^2 = \gamma_3^2 - x_{A3}^2$) we end up with $h = 2[(\gamma_3^2 - x_{A3}^2) + x_{A3}^2\mu]$. In case (iii), using that $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geq 0$ (due to $\gamma_1^2 \geq \gamma_2^2 = \gamma_3^2 - x_{A3}^2$) we have that $h = 2\{\gamma_1^2 + [\gamma_3^2 - \gamma_1^2 + (\gamma_1^2 - \gamma_3^2 + x_{A3}^2)\nu]\mu\}$, whose minimum occurs for $\mu = \nu = 0$ or $\mu = 1$ and $\nu = 0$ (depending on the sign of $\gamma_3^2 - \gamma_1^2$). Hence, even in cases (ii) and (iii), the minima of h fall on the boundary of \mathcal{S} . The above shows that no minima points at which h is differentiable can lie in the interior of \mathcal{S} .

Let us now address singular points, i.e., those at which h is non-differentiable and hence minimization criteria based on partial derivatives do not apply. These points (see above discussion) are the zeros of the function $f = a^2 - b$. Our aim is proving that even such points, if existing, lie on the boundary of \mathcal{S} . Firstly, note that $f \geq 0$ (we recall that $a^2 \geq b$ always holds, see Section II). This means that a zero of f is also a minimum point for f . From Eqs. (67)-(70) it is evident that $f(\mu, \nu)$ is analytic throughout the real plane. Then a necessary condition for this function to take a minimum is $\partial_\mu f = \partial_\nu f = 0$. It is easy to check that $\partial_\nu f$ is a simple second-degree polynomial in μ , with zeros $\mu_{s1} = 0$ and $\mu_{s2} = (\gamma_1^2 + \gamma_2^2 - 2\gamma_3^2 + 2x_{A3}^2)/[(\gamma_1^2 - \gamma_3^2 + x_{A3}^2) + (\gamma_2^2 - \gamma_1^2)\nu]$. The former solution clearly cannot correspond to stationary points of f – in particular zeros of f , i.e., *singular points of h* – that lie in the interior of \mathcal{S} (as anticipated, a zero of f is also a minimum and thus one of its stationary points). On the other hand, by plugging μ_{s2} into $\partial_\mu f$ we find $\partial_\mu f|_{\mu=\mu_{s2}} = 4(\gamma_1^2 - \gamma_3^2 + x_{A3}^2)(\gamma_2^2 - \gamma_3^2 + x_{A3}^2)$,

which vanishes for either $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 = 0$ or $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 = 0$. We have already shown (see above) that in neither of these two cases h can admit minima in the interior of \mathcal{S} .

B. Minima on the boundary of \mathcal{S}

The findings of the previous subsection show that we can restrict the search for the minimum of h to the boundary of \mathcal{S} . The possible values of h on the square edges corresponding to $\mu = 0, \mu = 1, \nu = 0$ and $\nu = 1$ are, respectively, given by

$$h_{\mu=0} = \gamma_1^2 + \gamma_2^2 + |\gamma_1^2 - \gamma_2^2| = 2\gamma_1^2, \quad (72)$$

$$h_{\mu=1} = \gamma_3^2 + x_{A3}^2 + \gamma_2^2 + (\gamma_1^2 - \gamma_2^2)\nu + |\gamma_2^2 - \gamma_3^2 + x_{A3}^2 + (\gamma_1^2 - \gamma_2^2)\nu|, \quad (73)$$

$$h_{\nu=0} = \gamma_2^2 + \gamma_1^2 - (\gamma_1^2 - \gamma_3^2 - x_{A3}^2)\mu + |\gamma_2^2 - \gamma_1^2(1-\mu) + (x_{A3}^2 - \gamma_3^2)\mu|, \quad (74)$$

$$h_{\nu=1} = \gamma_2^2 + \gamma_1^2 - (\gamma_2^2 - \gamma_3^2 - x_{A3}^2)\mu + |\gamma_1^2 - \gamma_2^2(1-\mu) + (x_{A3}^2 - \gamma_3^2)\mu|. \quad (75)$$

From Eq. (72) it trivially follows that the minimum of h on edge $\mu = 0$ is given by $\min h_{\mu=0} = 2\gamma_1^2$. In the next three dedicated paragraphs, we minimize h on edges $\mu = 1$ and $\nu = 0, 1$, respectively.

1. Edge $\mu = 1$

This is the set of points ($\mu = 1, 0 \leq \nu \leq 1$) on which function h is given by Eq. (73). Let h_+ (h_-) be the expression taken by h when the absolute value in Eq. (73) is positive (negative). These are easily calculated as

$$h_+(\nu) = 2[\gamma_2^2 + x_{A3}^2 + (\gamma_1^2 - \gamma_2^2)\nu], \quad h_-(\nu) = 2\gamma_3^2. \quad (76)$$

Importantly, note that h_+ always grows with ν while h_- is flat.

The argument of the absolute value [cf. Eq. (73)] increases with ν (since $\gamma_1^2 \geq \gamma_2^2$) and vanishes for $\nu = \nu_0 = -(\gamma_2^2 - \gamma_3^2 + x_{A3}^2)/(\gamma_1^2 - \gamma_2^2)$. Hence, it is negative (non-negative) for $\nu < \nu_0$ ($\nu \geq \nu_0$). As a consequence, $h = h_-$ ($h = h_+$) for $\nu < \nu_0$ ($\nu \geq \nu_0$). Now, the minimum of h on this edge depends on the sign of ν_0 , which depends in turn on the sign of $\gamma_2^2 - \gamma_3^2 + x_{A3}^2$. Indeed, if $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 < 0$ then $\nu_0 > 0$ and thus $\min h_{\mu=1} \equiv \min h_- = 2\gamma_3^2$ (recall that h_+ grows with ν). If, instead, $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 \geq 0$ then $\nu_0 \leq 0$ and $h \equiv h_+$ for $0 \leq \nu \leq 1$, namely throughout the edge. The minimum is thus taken at $\nu = 0$ and reads $\min h_{\mu=1} \equiv \min h_+(\nu=0) = 2(\gamma_2^2 + x_{A3}^2)$. To summarize,

$$\text{if } \gamma_2^2 - \gamma_3^2 + x_{A3}^2 < 0 \quad \min h_{\mu=1} = 2\gamma_3^2, \quad (77)$$

$$\text{if } \gamma_2^2 - \gamma_3^2 + x_{A3}^2 \geq 0 \quad \min h_{\mu=1} = 2(\gamma_2^2 + x_{A3}^2), \quad (78)$$

2. Edge $\nu = 0$

This is the set of points ($0 \leq \mu \leq 1, \nu = 0$), where h is given by Eq. (74). Similarly to the previous paragraph, we first search for the zero of the absolute value, which is easily found as $\mu = \mu_0 = (\gamma_1^2 - \gamma_2^2)/(\gamma_1^2 - \gamma_3^2 + x_{A3}^2)$. Its location on the real axis

fulfills

$$\text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geq 0 \begin{cases} \text{if } \gamma_2^2 - \gamma_3^2 + x_{A3}^2 \geq 0, & 0 \leq \mu_0 \leq 1, \\ \text{if } \gamma_2^2 - \gamma_3^2 + x_{A3}^2 < 0, & \mu_0 > 1, \end{cases} \quad (79)$$

$$\text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 < 0, \quad \mu_0 < 0, \quad (80)$$

which we will use in our analysis. At variance with the previous paragraph, now the absolute value in Eq. (74) grows (decreases) with μ for $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geq 0$ ($\gamma_1^2 - \gamma_3^2 + x_{A3}^2 < 0$). Eq. (73) straightforwardly gives

$$h_+(\mu) = 2(\gamma_2^2 + x_{A3}^2 \mu), \quad h_-(\mu) = 2[\gamma_1^2 + (\gamma_3^2 - \gamma_1^2)\mu], \quad (81)$$

where h_{\pm} are defined in full analogy with the previous paragraph. Note that, while h_+ always grows with μ , h_- is an increasing (decreasing) function of μ for $|\gamma_3| \geq |\gamma_1|$ ($|\gamma_3| < |\gamma_1|$). Let us analyze the possible situations. Based on the above, if $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geq 0$ then $\mu_0 \geq 0$ and, moreover, the absolute value is negative (non-negative) for $\mu < \mu_0$ ($\mu \geq \mu_0$). This

yields $h(\mu < \mu_0) = h_-$ and $h(\mu \geq \mu_0) = h_+$. Now, two cases can occur. If $|\gamma_3| \geq |\gamma_1|$, then h_- grows with μ and therefore $\min h_{v=0} \equiv h_-(\mu=0) = 2\gamma_1^2$. If $|\gamma_3| < |\gamma_1|$, instead, h_- decreases with μ . Then the minimum of h depends on whether or not $\mu_0 \leq 1$, which depends in turn on the sign of $\gamma_2^2 - \gamma_3^2 + x_{A3}^2$ according to Eq. (79). If $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 \geq 0$ then $\mu_0 \leq 1$ and h is minimized for $\mu = \mu_0$ (recall that h_+ always grows). This yields $\min h_{v=0} \equiv h_-(\mu_0) = 2[\gamma_1^2(\gamma_2^2 + x_{A3}^2) - \gamma_2^2\gamma_3^2]/(\gamma_1^2 - \gamma_3^2 + x_{A3}^2)$. On the other hand, $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 < 0$ implies $\mu_0 > 1$. Hence, $h \equiv h_-$ throughout the interval $0 \leq \mu \leq 1$ and, necessarily, $\min h_{v=0} \equiv h_-(\mu=1) = 2\gamma_3^2$.

We are left with the case $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 < 0$. In this situation, $\mu_0 < 0$ [cf. Eq. (80)] and the absolute value is non-negative (negative) for $\mu \leq \mu_0$ ($\mu > \mu_0$), which gives $h \equiv h_-$ throughout this edge. Now, the analysis is simpler since, evidently, only the case $|\gamma_1| < |\gamma_3|$ is possible. Thus h_- can only increase [recall Eq. (81)] and $\min h_{v=0} = h_-(\mu=0) = 2\gamma_1^2$.

To summarize, on the edge $v=0$

$$\text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 < 0 \quad \min h_{v=0} = 2\gamma_1^2, \quad (82)$$

$$\text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geq 0 \begin{cases} \text{if } |\gamma_3| \geq |\gamma_1| & \min h_{v=0} = 2\gamma_1^2, \\ \text{if } |\gamma_3| < |\gamma_1| & \min h_{v=0} = \Theta(\gamma_2^2 - \gamma_3^2 + x_{A3}^2) 2 \frac{\gamma_1^2(\gamma_2^2 + x_{A3}^2) - \gamma_2^2\gamma_3^2}{\gamma_1^2 - \gamma_3^2 + x_{A3}^2} + \Theta[-(\gamma_2^2 - \gamma_3^2 + x_{A3}^2)] 2\gamma_3^2 \end{cases} \quad (83)$$

3. Edge $v=1$

This is the set of points ($0 \leq \mu \leq 1$, $v=1$), where h is given by Eq. (75). Similarly to the previous paragraph, we first search for the zero of the absolute value, which is easily found as $\mu = \mu_0 = -(\gamma_1^2 - \gamma_2^2)/(\gamma_2^2 - \gamma_3^2 + x_{A3}^2)$. Its location on the real axis fulfills

$$\text{if } \gamma_2^2 - \gamma_3^2 + x_{A3}^2 \geq 0 \quad \mu_0 \leq 0, \quad (84)$$

$$\text{if } \gamma_2^2 - \gamma_3^2 + x_{A3}^2 < 0 \begin{cases} \text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geq 0 & 0 < \mu_0 \leq 1 \\ \text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 < 0 & \mu_0 > 1 \end{cases} \quad (85)$$

Based on Eq. (75), the expressions taken by h on this edge when the absolute value is positive and negative are, respectively

$$h_+(\mu) = 2(\gamma_1^2 + x_{A3}^2 \mu), \quad h_-(\mu) = 2[\gamma_2^2 + (\gamma_3^2 - \gamma_2^2)\mu]. \quad (86)$$

Hence, h_+ always grows with μ while h_- is an increasing (decreasing) function of μ for $|\gamma_3| \geq |\gamma_2|$ ($|\gamma_3| < |\gamma_2|$). We show next that, the minimum of h on this edge is always given by $2\gamma_1^2$.

Indeed, if $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 \geq 0$ (implying $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geq 0$) then $\mu_0 \leq 0$ and $h \equiv h_+(\mu)$ throughout the edge. The minimum is

thus $\min h_{v=1} = h_+(0) = 2\gamma_1^2$. If, instead, $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 < 0$ then $h = h_+$ ($h = h_-$) for $\mu \leq \mu_0$ ($\mu > \mu_0$). Moreover, note that in this case one has $\gamma_3^2 > \gamma_2^2$, which entails [cf. Eq. (86)] that both h_- and h_+ grow with μ . Hence, the minimum is again given by $\min h_{v=1} = h_+(0) = 2\gamma_1^2$, which completes our proof.

C. Global minimum

To give the general expression for the minimum of h it is convenient to refer to the minimization study on the edge $v=0$. Recall that the minimum of h on the edges $\mu=0$ and $v=1$ is *unconditionally* given by $2\gamma_1^2$. When $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 < 0$, based on Eqs. (77) and (82) the minimum reads $\min_e h = 2\gamma_1^2$ (note indeed that this case necessarily entails $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 < 0$ and $\gamma_1^2 < \gamma_3^2$). If instead $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geq 0$, both signs of $\gamma_1^2 - \gamma_3^2 + x_{A3}^2$ as well as $|\gamma_3| - |\gamma_1|$ are possible. Hence, if $|\gamma_3| \geq |\gamma_1|$ upon analysis of Eqs. (77), (78) and the first case in Eq. (83) we end up with $\min_e h = \min\{2\gamma_1^2, 2(\gamma_2^2 + x_{A3}^2)\}$. For $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 < 0$, this gives $\min_e h = 2\gamma_3^2$. For $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 \geq 0$, the global minimum is the lowest number among $2\gamma_1^2$, $2(\gamma_2^2 + x_{A3}^2)$ and $2[\gamma_1^2(\gamma_2^2 + x_{A3}^2) - \gamma_2^2\gamma_3^2]/(\gamma_1^2 - \gamma_3^2 + x_{A3}^2)$. Hence, to summarize,

$$\begin{aligned}
& \text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 < 0 \quad \min h = 2\gamma_1^2, \\
& \text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geq 0 \quad \begin{cases} \text{if } |\gamma_3| \geq |\gamma_1| & \min h = \Theta(\gamma_2^2 - \gamma_3^2 + x_{A3}^2) 2 \min \left\{ \gamma_1^2, \gamma_2^2 + x_{A3}^2 \right\} + \Theta \left[-(\gamma_2^2 - \gamma_3^2 + x_{A3}^2) \right] 2\gamma_1^2, \\ \text{if } |\gamma_3| < |\gamma_1| & \min h = \Theta(\gamma_2^2 - \gamma_3^2 + x_{A3}^2) 2 \min \left\{ \gamma_1^2, \gamma_2^2 + x_{A3}^2, \frac{\gamma_1^2(\gamma_3^2 + x_{A3}^2) - \gamma_2^2\gamma_3^2}{\gamma_1^2 - \gamma_3^2 + x_{A3}^2} \right\} + \Theta \left[-(\gamma_2^2 - \gamma_3^2 + x_{A3}^2) \right] 2\gamma_3^2. \end{cases}
\end{aligned} \tag{87}$$

Eq. (87) can be further simplified. Indeed, on the second line (case $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geq 0$ and $|\gamma_3| \geq |\gamma_1|$) for $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 \geq 0$ we have $\gamma_2^2 + x_{A3}^2 \geq \gamma_3^2 \geq \gamma_1^2$ and therefore the minimum is $2\gamma_1^2$ regardless of $\gamma_2^2 + x_{A3}^2 \geq \gamma_3^2$. On the other hand, on the third line (case $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geq 0$ and $|\gamma_3| < |\gamma_1|$) for $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 \geq 0$ and using $\gamma_1^2 \geq \gamma_2^2$ it is straightforward to prove that the rational function can never exceed both γ_1^2 and $\gamma_2^2 + x_{A3}^2$. In light of these considerations and upon comparison of Eq. (87) with Eqs. (82) and (83), we conclude that the global minimum of h is achieved on the edge $\nu = 0$. Therefore, using Eq. (32) the TDD of an arbitrary two-qubit X state is finally obtained as in Eq. (65). Remarkably, in each case that can occur (depending on the parameters defining the state) $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$ takes a relatively compact expression.

As already anticipated, for Bell-diagonal states (see Section III), Eq. (65) yields the result of Section III A as shown in detail in Appendix B.

Another interesting special case occurs when in Eq. (63) either $\rho_{32} = 0$ or $\rho_{41} = 0$. Then, due to Eq. (64), $|\gamma_1| \equiv |\gamma_2|$ and $\sqrt{\frac{\gamma_1^2(\gamma_2^2 + x_{A3}^2) - \gamma_2^2\gamma_3^2}{\gamma_1^2 - \gamma_3^2 + x_{A3}^2}} \rightarrow \frac{|\gamma_2|}{2}$. Hence, such a case always entails $\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = |\gamma_1|/2$, namely half of the absolute value of the non-zero off-diagonal entry.

VI. CONCLUSIONS

In this paper, we have addressed the issue of the computability of TDD, one of the most reliable and advantageous QCs indicators. By introducing a new method for tackling and simplifying the minimization required for its calculation in the two-qubit case, we have demonstrated that this can be reduced to the search for the minimum of an explicit two-variable function. Then, we have shown that this can be analytically found in a closed form for some relevant classes of states, which encompass arbitrary quantum-classical and X states. The latter includes as a special subset the Bell diagonal states, which were the only states for which an analytical expression of TDD had been worked out prior to our work.

Due to the importance of quantum-classical and X states, along with the typical hindrances to the calculation of their QCs through bona fide measures, our work provides a significant contribution to the study of QCs quantifiers, by combining the desirable mathematical properties of TDD with its explicit computation for these classes of density matrices. Furthermore, we expect that the framework developed in this pa-

per may be further exploited in future investigations to enlarge the class of quantum states that admit an analytical expression for TDD.

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Appendix A: Derivation of Eq. (48)

We recall that $f_{\pm}(\phi, \alpha) = \gamma \cos \phi \pm x_A \cos(\phi - \alpha)$. This is a linear combination of $\cos \phi$ and $\sin \phi$, which can be arranged in terms of a single cosine as $A_{\pm}(\cos \phi \cos \delta_{\pm} + \sin \phi \sin \delta_{\pm}) = A_{\pm} \cos(\phi - \delta_{\pm})$. Using $\tilde{x}_{A1} = x_A \cos \alpha$ [see Eq. (44)], the factor is easily found as $A_{\pm} = \sqrt{(\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2}$, while

$$\sin \delta_{\pm} = \frac{\pm x_A \sin \alpha}{\sqrt{(\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2}} = \frac{\pm \tilde{x}_{A2}}{\sqrt{(\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2}} \tag{A1}$$

$$\cos \delta_{\pm} = \frac{\gamma \pm x_A \cos \alpha}{\sqrt{(\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2}} = \frac{\gamma \pm \tilde{x}_{A1}}{\sqrt{(\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2}}. \tag{A2}$$

Hence, $\delta_{\pm} = \arctan[\tilde{x}_{A2}/(\tilde{x}_{A1} \pm \gamma)]$. Therefore

$$f_{\pm}(\phi, \alpha) = \sqrt{(\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2} \cos(\phi - \delta_{\pm}). \tag{A3}$$

Replacing Eq. (A3) into Eq. (47) of the main text yields

$$\begin{aligned}
\|M(\hat{\rho})\|_1 &= 2 \sum_{\eta=\pm} \sqrt{[(\gamma + \eta \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2] [1 - \cos^2(\phi - \delta_{\eta})]} \\
&= 2 \sum_{\eta=\pm} \sqrt{(\gamma + \eta \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2} |\sin(\phi - \delta_{\eta})| \\
&= 2 \sum_{\eta=\pm} \sqrt{(\gamma + \eta \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2} |\sin \phi \cos \delta_{\eta} - \cos \phi \sin \delta_{\eta}|.
\end{aligned}$$

Eliminating now $\sin \delta_{\pm}$ and $\cos \delta_{\pm}$ through Eqs. (A1) and (A2) we end up with Eq. (48) of the main text.

Appendix B: Eq. (65) for Bell diagonal states

Bell diagonal states are defined as a mixture of the four Bell states. This immediately yields that they fulfill $\vec{x}_A = \vec{x}_B = 0$, that is, the reduced density matrix describing the state of either party is maximally mixed. Therefore, the corresponding density matrix can be expanded as a linear combination of $\mathbb{1}_A \otimes \mathbb{1}_B$ and $\{\sigma_{Ak} \otimes \sigma_{Bk}\}$. As each of these four operators has an X -form matrix representation [cf. Eq. (63)] Bell-diagonal states are X states. Hence, in Eq. (65) $\gamma_i^2 - \gamma_3^2 + x_{A3}^2 \rightarrow \gamma_i^2 - \gamma_3^2$ for $i = 1, 2$. In this case, the square root in Eq. (65) coincides with

$|\gamma_2|$ and the TDD reduces to

$$\begin{aligned} |\gamma_3| \geq |\gamma_1| &\Rightarrow \mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{|\gamma_1|}{2}, \\ |\gamma_3| < |\gamma_1| &\Rightarrow \mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{1}{2} \max\{|\gamma_2|, |\gamma_3|\} \end{aligned} \quad (\text{B1})$$

It is immediate to check that the above is equivalent to state that $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$ is half of the *intermediate* value among $\{|\gamma_1|, |\gamma_2|, |\gamma_3|\}$, which fully agrees with Refs. [12, 13] and the findings of Sec. III A.

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